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AWS Cloud

HECC AWS Cloud: Overview

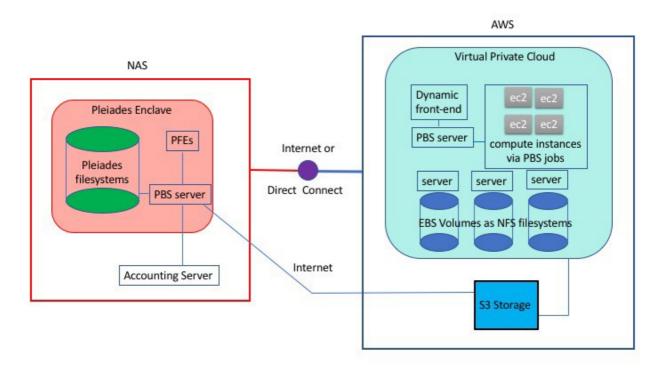
Starting summer 2019, we now offer the Amazon Web Services (AWS) Cloud on a pay-for-use basis. If you are a principal investigator (PI) directly affiliated with NASA, and you are interested in paying with NASA funding to use AWS Cloud for your projects, please contact us at support@nas.nasa.gov. Access to the AWS Cloud for users in a PI's project will be granted after funding is received and the AWS environment is configured for the PI's project.

Webinar: In addition to the articles in this section, you can find more information in our user training webinar, "Overview of HECC Pay-for-Use AWS Cloud." The recording and presentation slides are available in the <u>HECC webinars archive</u>.

This article provides a high-level overview of the HECC AWS Cloud. Follow the links in each section to learn more details about using the AWS Cloud.

HECC AWS Cloud Environment

As shown in this diagram, a project's HECC AWS Cloud environment includes both the HECC resources located at the NAS facility, and HECC's AWS resources. The resources at NAS are shared among projects, while those at AWS are private for each project. Some of the resources are optional, depending on the need of a project.



NAS-Located Resources

The purpose and functions of the NAS-located resources are described in this section.

AWS Cloud 1

Pleiades Front-End Systems (PFEs)

Each user in a project must have a NAS account in order to log in to a PFE. Access to AWS resources is accomplished via an SSH session from a PFE. Authentication to AWS is done behind the scenes.

From a PFE, you can remotely manage:

- PBS jobs submitted to AWS
- Data stored in AWS S3 storage

NAS PBS Server

A PBS server located at NAS, currently called clpbs-01, is used for accepting and checking PBS jobs submitted to run on AWS.

Pleiades /nobackup Filesystems

To run a job from NAS, you must submit it to AWS from your Pleiades /nobackup filesystem. The PBS output/error files of the AWS batch jobs are sent back to the \$PBS_O_WORKDIR on your /nobackup filesystem.

Your /nobackup filesystem is also one of the sources or destinations for <u>different types of file</u> <u>transfers between NAS and AWS</u>.

Accounting Server

The accounting server manages your cloud allocations in <u>Cloud Billing Units (CBUs)</u>. You can check your cloud allocation and usage by running the NAS acct ytd and acct query tools.

AWS Resources

The purpose and functions of the AWS resources are described in this section.

Note: The term *instance* used at AWS is logically equivalent to the term *node* used at NAS.

Dynamic Front End

In order to save costs, there is no static front end for AWS that runs 24x7. Instead, you launch a <u>dynamic front end</u> when you need one, and then shut it down when you're done. You only pay for the time that the dynamic front end is running.

A dynamic front end uses one AWS Elastic Compute Cloud (EC2) instance of your choice.

Use the dynamic front end to compile applications, and/or to manage and check PBS jobs or data on AWS. A limited number of software modules are available in the /nasa directory; if you need additional software, you must install it yourself under your own directory.

For more information, see AWS Elastic Compute Cloud (EC2) instance types.

AWS PBS Server

The PBS server at AWS coordinates with the PBS server at NAS to manage:

- Batch jobs submitted remotely from a PFE
- Batch jobs submitted locally from a dynamic front end

Note: Be sure to read <u>AWS PBS Resources and Examples</u> before submitting a batch job to AWS.

To save costs, the AWS PBS server is shut down when there are no batch jobs to manage.

The hostname of the AWS PBS server is different for each project. To find yours, use the following script on a PFE:

/u/scicon/tools/bin/aws pbs host

If you have multiple AWS projects, each with its own PBS server, add --group gid to the aws_pbs_host command to find the PBS server associated with that GID.

The instance type used for the server is currently m5.xlarge. It may change in the future.

Compute Instances for Batch Jobs

AWS offers many types of EC2 instances that you can use to run batch jobs. The default regions are **US West** for public cloud and **AWS GovCloud (US)** for government cloud. The HECC AWS Cloud uses the Linux AMI operating system.

Pricing varies with regions and operating systems.

For more information, see:

- EC2 instance types
- EC2 pricing
- EC2 regions and availability zones

Filesystem Servers

A filesystem requires a server with sufficiently high bandwidth to the filesystem. A c5.18x instance (similar to an Electra Skylake node) is typically chosen for the persistent filesystem described below. For a job-time filesystem, the instance chosen varies depending on the size to be allocated to the filesystem. For example:

- A c5d.18x instance for sizes below 1.8 terabyte (TB)
- An h1.16x instance for sizes above 4 TB and below 16 TB
- A c5.18x instance with Elastic Block Store (EBS) for all other sizes

To save costs, the server is shut down when the filesystem is not in use. If you need multiple filesystems, then you will need multiple servers.

Electric Block Store (EBS) Volumes as Filesystems

You can use Electric Block Store (EBS) Volumes as filesystems. AWS offers several EBS volume types and pricing. Depending on your project's need, different volumes can be provisioned into two types of filesystems:

• A persistent filesystem is independent of a batch job. Data in the filesystem persists even when the filesystem is not used. You pay for the persistent cost of the size provisioned, and for the time when the filesystem server is running.

This type of filesystem is usually configured by HECC staff upon your request at the beginning of your project.

• A <u>job-time filesystem</u> is created at the beginning of a batch job and terminated at the end of the job. The data in this filesystem is lost at the end of the job. You pay for the size provisioned for the lifetime of the job, and the uptime of the filesystem server (if needed). Some job-time filesystems might not use EBS volumes.

For more information, see:

- EBS volumes
- EBS volume types
- EBS pricing

S3 (Simple Storage Service) for Long-Term Storage

Among the multiple S3 (Simple Storage Service) classes offered by AWS, HECC uses the standard class. Pricing depends on space used, the frequency of request, and the amount of data transferred out of S3 to the Internet. For more information, see:

- S3 storage classes
- S3 pricing

AWS Cloud File Transfer Overview

This article provides a high-level view of available methods for file transfers among various NAS and Amazon Web Services (AWS) filesystems or storage systems.

Transferring Files Between NAS and AWS Systems

Transfers Between Your PFE /home or /nobackup Filesystem and an AWS Persistent Filesystem

To use these methods, you must have a configured persistent filesystem and the IP address of a live <u>AWS dynamic front end</u>.

Option 1: Initiate Transfer from a PFE by Using scp

To transfer your file:

```
pfe% scp -i \sim/.ssh/id_rsa_yours iii.jjj.kkk.lll:/nobackup/your_user_name/filename . pfe% scp -i \sim/.ssh/id_rsa_yours -r src iii.jjj.kkk.lll:/nobackup/your_user_name
```

Replace id_rsa_yours with the name of the RSA private key file that is set up for you to connect to AWS under your Pleiades .ssh directory, and replace iii.jjj.kkk.lll with the actual IP address of your live AWS dynamic front end.

Option 2: Initiate Transfer from the AWS Dynamic Front End by Using sup + shiftc

Before you can use this method, follow the instructions in <u>Downloading SUP to Enable Remote Transfers</u> to install **sup** into your AWS ~/**bin** directory.

To transfer your file:

```
aws% which sup
~/bin/sup
aws% sup shiftc pfe21.nas.nasa.gov:~/file1 .
```

sup + shiftc will choose a transfer protocol for you based on what's available in your AWS environment. You can also specify a transfer protocol explicitly, for example, scp, as follows:

```
aws% sup scp file2 pfe21.nas.nasa.gov:
```

Note: You will need to provide your NAS password and PIN+passcode to generate the SUP authentication key, which is valid for 7 days.

Option 3: Initiate Transfer from the AWS Dynamic Front End by Using scp

Before you can use this method, you must set up <u>SSH passthrough</u> to allow one-step login from AWS to a PFE.

Note: You will need to modify the NAS-provided config file in order to get it working on the HECC

AWS Cloud. Modify the file by replacing Host *.nas.nasa.gov with Host pfe*.nas.nasa.gov lfe*.nas.nasa.gov.

To transfer your file:

aws% scp file2 pfe21.nas.nasa.gov:

Transfers Between Your PFE /home or /nobackup Filesystem and AWS S3

All users have space under their project's S3 storage. You can use the following set of nas_s3_xxx
commands on a PFE to view, transfer, and delete files and directories under your S3 root location:

View: nas_s3_ls

• Transfer: nas_s3_put and nas_s3_get

• Delete: nas_s3_del

Read <u>this article</u> for more information.

Transfers Between your PFE /nobackup Filesystem and an AWS Filesystem Accessible from a PBS Job

Through a PBS job submitted from your Pleiades /nobackup directory, you can add directives to stagein or stageout files or directories to/from the job's \$PBS_O_WORKDIR on AWS. The \$PBS_O_WORKDIR could be on a persistent filesystem or a <u>job-time filesystem</u>, depending on the set up of the PBS job.

The available directives are:

```
#CLOUD -stagein_file=path_to_file/file
#CLOUD -stagein_dir=path_to_dir
#CLOUD -stageout_file=path_to_file/file
#CLOUD -stageout_dir=path_to_dir
#CLOUD -stageout_file_delete=output
```

Read this article for more information.

Transferring Files within AWS

Transfers Between S3 and the Dynamic Front End

You can use the set of <code>nas_s3_xxx</code> commands on an AWS dynamic front end to view, transfer, and delete files and directories under your S3 root location:

View: nas_s3_ls

Transfer: nas_s3_put and nas_s3_get

• Delete: nas s3 del

Read <u>this article</u> to find more information.

Transfers Between S3 and \$PBS_O_WORKDIR within a PBS Job

You can use the following directives to copy files between your \$PBS_O_WORKDIR on AWS and your S3 storage on AWS.

Note: \$PBS_O_WORKDIR could physically be on a persistent or a job-time filesystem on AWS.

```
#CLOUD -get_file=path_to_file/file
#CLOUD -get_file=sub_dir/file:upper_dir
#CLOUD -get_dir=path_to_dir
#CLOUD -get_dir=sub_dir:upper_dir
#CLOUD -put_file=src:optional_dest_dir
#CLOUD -put_dir=src_dir:optional_dest_dir
```

Read this article for more information.

Transfers Between S3 and Job-Time Filesystems within a PBS job

You can use these directives to copy files between a job-time filesystem and your S3 storage on AWS.

```
#CLOUD -volume_get=s3_folder_to_copy_data_from
#ClOUD -volume_put=s3_folder_to_save_data_to
```

Read this article for more information.

AWS Dynamic Front End

Because there is no static front end for AWS, you launch a dynamic front end only when you need one, and then shut it down when you're done. You only pay for the time that the front end is running.

This article provides instructions for launching, accessing, and terminating an AWS dynamic front end from a Pleiades front end (PFE), along with some basic usage information.

Launching a Dynamic Front End

To launch a dynamic front end, run the aws_fe command from a PFE to start an instance, as shown below. This command creates a batch job that runs behind the scenes to request the resources. There is no limit on the number of AWS front ends you can request or run.

```
pfe% /u/scicon/tools/bin/aws fe -h
aws fe (optional resource specs)
will start a front end for the user in AWS that will run for a default 1 hour and have 1 core
       --group X
                     Charge against the given group. (Your default cloud group is scicon)
       --region X
                      Launch in the given region if the project supports multiple regions
       --container X Enable the given container technology enabled. Current options: singularity
       --jupyter
                     Create a front end instance with a jupyter notebook running.
       --jupyterlab
                     Create a front end instance with a jupyter lab running.
                     Request X hours of walltime
-t X (--hour X)
-c X (--cores X)
                     Create instance with at least X cores
-m X (--mem X)
                      Create instance with at least X G of ram
-g X (--gpu X)
                     Create instance with the specified GPU type attached. Options: v100/a100/k80
-n X (--ngpu X)
                     Request X cards of the specified type in the instance
-a X (--arch X)
                     Request the 'X' model of instances, not valid with -g/--gpu.
                           Options: m4/m5/c4/c5/c5a
-1
     (--list)
                     Print login instructions for the existing front end instance the user has,
                          should one exist
     (--kill)
-k
                     Terminate an existing front end instance. If only 1 FE exists it will be killed.
                          If multiple FEs exist it returns an error unless -j is also used.
-j X (--job X)
                      When used with --kill will kill the FE with the given ID.
                          See output from --list for the value of ID for each front end.
      (--dcv)
                      Create a front end with DCV running, instructions on logging in will be emailed
      (--shared)
                      Allows all users in the same group to be able to use the DCV gui as well
-b X (--band X)
                     Request X amount of network bandwidth per instance. Options: 1/10/25 (Gbps)
                           Note that using this option with others can result in an impossible
                           combination of options.
                           The request will fail silently
```

The following PDFs list the CPU and GPU node types that are supported in AWS:

- CPU node types (PDF)
- GPU node types (PDF)

Recommendation: For your convenience, include /u/scicon/tools/bin in your PATH so that aws_fe can be found without including the full path in the command line. You can also accomplish this by loading a module on a PFE:

```
module load /u/scicon/tools/modulefiles/scicon_cli_tools
```

If you have more than one cloud project group ID (GID), one of them will be used as a default for aws_fe as listed in the output of aws_fe -h. Use the --group option to specify a non-default cloud GID. If you want to change your default cloud GID, send an email to support@nas.nasa.gov to open a ticket.

Running the aws_fe command without any arguments will launch a front end consisting of 1 node, with at least 8 GB of memory and 1 CPU core, that will remain for 1 hour.

Note: The current default instance type assigned is m5.xlarge, which has 2 cores and 16 GB, and costs \$0.192/hour in the US West public cloud. The default may be different for your project.

Example: Launch an Instance with a K80 GPU

This example launches an instance that has at least one K80 GPU on it:

```
pfe% aws_fe -l
No front end to display

pfe% aws_fe -t 4 -g k80 -n 1
The front end is booting, when the instance is ready an email will be sent to your NAS email with login instructions.
```

Sample Email Confirmation

If your launch is successful, you will receive an email similar to the following to confirm that the instance has started and provide login instructions:

```
Your front end instance has started in AWS.

To log in use the following from a PFE machine:
env SSH_AUTH_SOCK="" ssh -i ~/.ssh/id_rsa_yours your_nas_username@iii.jjj.kkk.lll
```

Note: If you don't see an email a few minutes after launching, check your email spam folder. This is likely to happen for users who forward their NAS emails to (or through) Gmail.

TIP: If your PBS server at AWS is asleep, your first launch attempt might fail. If this happens, you will receive an email with the message "Job rejected by all possible destinations." This first failed attempt will wake up the PBS server; you can then repeat the aws_fe command to try launching the instance again.

Accessing a Dynamic Front End

To access a dynamic front end, run SSH from a PFE, as shown below.

Note: The first time you access the assigned front end, you might be prompted with the question: Are you sure you want to continue connecting (yes/no)?. Type yes.

```
pfe% env SSH_AUTH_SOCK="" ssh -i ~/.ssh/id_rsa_yours your_nas_username@iii.jjj.kkk.lll The authenticity of host 'iii.jjj.kkk.lll (iii.jjj.kkk.lll)' can't be established. ECDSA key fingerprint is SHA256:oE1wd9e/vGwo4cPj6oHwF182II1jo2p3H8gaSXBXGoY. Are you sure you want to continue connecting (yes/no)? yes -bash-4.2$
```

where *id_rsa_yours* is the one that was set up under your Pleiades .ssh directory for connecting to AWS, and *iii.jjj.kkk.lll* is the IP address of your live dynamic front end.

The front end host key is regenerated each time a new front end is started. This invalidates the copy in your Pleiades ~/.ssh/known_hosts file, which has the IP address used by a previous front-end node or compute node. When this happens, you will see a message similar to the following:

```
The fingerprint for the ECDSA key sent by the remote host is SHA256:4QGzjDB+xiYq3liOyC5Ymbmw4GbuMblcKKdwrV0rjYE. Please contact your system administrator. Add correct host key in /homeX/username/.ssh/known_hosts to get rid of this message. Offending ECDSA key in /homeX/username/.ssh/known_hosts:4 ECDSA host key for iii.jjj.kkk.lll has changed and you have requested strict checking. Host key verification failed.
```

If you see this message, you must modify your .ssh/known_hosts file on the PFE to remove the host key entry with the IP number from your new aws_fe request, and retry the SSH connection.

Once you are in, be aware that:

The default shell is bash.

```
[username@awsfe-XXXXX ~] echo $0 -bash
```

To change to csh for the current shell, do:

```
[username@awsfe-XXXXX ~] csh
[username@awsfe-XXXXX ~] echo $0
csh
```

To change to csh permanently on all AWS machines, send an email to support@nas.nasa.gov with your username and the GID(s) used on your AWS cloud environment.

- There is only a minimal .bashrc file set up for you. You should create your own startup scripts or modify the minimal .bashrc file to set variables such as \$PATH, or to load certain modules if your job relies on loading them inside a startup file.
- There is a limited number of software modules installed under the <code>/nasa</code> directory. Use the command <code>module avail</code> to see what is available. If you need a program that is not already available, you will have to install under your own directory.

Terminating the Dynamic Front End

When you are done using the dynamic front end, you must terminate it. If you simply exit the front end, it is still owned by youâ and you will continue to pay for itâ until either it reaches the wall-time limit specified at start time, or you terminate it by using one of the following methods:

• Use the -k option of aws fe command (recommended method):

```
pfe% aws fe -k [-j X]
```

Note: Include $-\mathbf{j}$ X if you have more than one front end running. You can find X from the output of aws_fe -1.

• Delete it using the aws_qdel command described in this article.

After you terminate the front end, you will receive an email with the front end usage statistics. (Check your spam folder if you do not see one.) Here is an example:

```
Job Resource Usage Summary for 3563.clpbs-01.nas.nasa.gov
Total Runtime : 00:59:46
Job Startup Time : 00:02:04
Time Spent In PBS Script : 00:57:41
Walltime Requested : 01:00:00
Charged To : cstaff
Job Finished : Wed Jul 3 14:37:29 2019
Instance Types (ondemand): 1 m5.xlarge
```

EBS Usage NAS overhead charge Job Costs : 8577331200 bytes : 0.000 percent : \$0.192358499543

Building and Running Applications in the AWS Cloud

This article provides basic information on building and running applications in the HECC AWS Cloud.

Due to differences in the operating systems and software stacks, an executable built on Pleiades will not run in the AWS Cloud. For information on transferring source files from Pleiades before building your executable in your AWS Cloud environment, see <u>AWS Cloud: File Transfer</u> Overview.

Available Modules

This list shows the default set of software packages installed under the /nasa directory in your AWS environment:

- Intel compiler
- PGI compiler
- Intel MPI
- OpenMPI
- CUDA

You (or NAS staff) can also install Python from the Intel or Conda distributions, if needed.

If you need any other software packages, you must install them into a non-root-privileged filesystem yourself. If you need a licensed software package, you must provide the license on your own.

Building and Running MPI Applications

The HPE MPT library is not available in your AWS Cloud environment. Use either Intel MPI or OpenMPI instead.

WARNING: The variable StrictHostKeyChecking is set to no in a system level configuration file, since both Intel MPI and OpenMPI rely on running SSH before launching an MPI process. If you reset this variable to yes or ask in your .ssh/config file, your MPI job will stall.

Using Intel MPI

Load an Intel MPI module in your build and run sessions. For example:

```
aws% module load intel-mpi/2019.3.062
```

To compile, load either an Intel compiler or a PGI compiler. This example uses an Intel compiler:

```
aws% module load comp-intel/2019.3.062 aws% mpiifort your_program.f aws% mpiicc your_program.c
```

If you use a PGI compiler, replace mpiifort with mpif90 and mpiicc with mpicc.

To run, use mpiexec in an interactive session or a PBS batch script:

```
mpiexec -np xx ./a.out
```

Using OpenMPI

In your system startup script, such as .bashrc or .profile (for bash) and .cshrc (for csh), include loading of an OpenMPI module. For example:

```
module load openmpi/4.0.1
```

This is needed if you plan to run OpenMPI executables across nodes.

To build an executable, use either an Intel compiler or a PGI compiler. This example uses a PGI compiler:

aws% module load comp-pgi/19.04 aws% mpif90 your_program.f aws% mpicc your_program.c

To run, use mpiexec in an interactive session or a PBS batch script:

mpiexec -np xx ./a.out

Managing AWS PBS Jobs Launched From a PFE

This article provides information on managing your Amazon Web Services (AWS) PBS jobs submitted from a Pleiades front end (PFE).

The PBS server at NAS for managing AWS cloud job is clpbs-01. It coordinates with another PBS server at AWS to get your job burst into and running on AWS, and sending the PBS output/error file back to Pleiades.

Note: The aws_pbs_host, aws_qstat, and aws_qdel scripts described in this article are located under the directory /u/scicon/tools/bin on Pleiades. The instructions below assume that you have included /u/scicon/tools/bin in your \$PATH.

Finding Available Queues

To find available queues, type the command:

```
pfe% qstat -q @clpbs-01
```

Among the queues listed in the output, you only have direct access to the *cloud* queue. The other queues, such as *frontend* and *s3op*, are used by NAS-controlled scripts (*aws_fe* and *nas_s3_xxx*) for managing the <u>AWS dynamic front end</u> and <u>data at AWS S3</u> on your behalf.

The limits of each queue are configured in the PBS server at AWS. To see them, use:

```
pfe% aws_qstat -Q @`aws_pbs_host` pfe% aws_qstat -Q @`aws_pbs_host --group gid` (to check for a non-default GID)
```

Note: If you get the following message, your PBS server at AWS has likely gone to sleep, for cost saving purposes. Submitting a job or two should wake up your server.

```
Connection timed out qstat: cannot connect to server your_aws_pbs_server.nas.nasa.gov (errno=110)
```

Submitting Jobs (qsub)

You must submit jobs to AWS from your Pleiades /nobackup filesystem.

From a PFE, you can submit regular batch jobs to the *cloud* queue, but not interactive jobs, using the following command:

```
pfe% qsub -q cloud@clpbs-01 job_script
```

To submit jobs to a non-default AWS GID, add the-W group_list=gid option, where gid is in the form of zxxxx (i.e., the letter "z" followed by four numbered digits):

```
pfe% qsub -q cloud@clpbs-01 -W group_list=gid job_script
```

or add it inside your PBS script:

```
#PBS -W group_list=gid
```

Note: If you get the following message within a few minutes of submitting your job, your PBS server at AWS likely went to sleep, for cost saving purposes; however, by this time it should have been awakened and subsequent jobs should go through.

```
PBS Job Id: xxxx.clpbs-01.nas.nasa.gov
Job Name: test.pbs
Aborted by PBS Server
Job rejected by all possible destinations
```

Checking Jobs (qstat or aws_qstat)

When a job is submitted from a PFE, it is under the control of the PBS server clpbs-01 at the beginning, and running qstat at that time on a PFE will show the job.

```
pfe% qstat -a @clpbs-01
```

The status of a job is H (held) while any files are copied to temporary storage on the AWS cloud. When the copy is completed, the status changes to M, indicating that it was moved to the PBS server at AWS. The job then disappears from clpbs-01. However, you can see past jobs using the following:

```
pfe% qstat -x @clpbs-01
```

After clpbs-01 hands over the control for the job to AWS, the job is visible from your AWS PBS server, using:

```
pfe% aws_qstat @`aws_pbs_host`
pfe% aws_qstat @`aws_pbs_host --group gid` (to check for a non-default GID)
```

You can get more detailed information about a job using the following:

```
pfe% aws_qstat -f jobid.clpbs-01.nas.nasa.gov@`aws_pbs_host --group gid`
```

When a job finishes, it may take a few minutes for the PBS output file to show up in your Pleiades directory. You can check whether your job has completed using:

```
pfe% aws_qstat -xqst @`aws_pbs_host --group gid`
```

Deleting Jobs (aws_qdel)

To delete jobs submitted to AWS from a PFE, use the script aws_qdel. Note that you cannot delete these jobs using the standard qdel command, because it involves the coordination of two PBS servers.

```
pfe% aws_qdel jobid
or
pfe% aws qdel jobid.clpbs-01.nas.nasa.qov
```

To delete a job for a non-default AWS GID, use:

```
pfe% aws_qdel --group gid jobid
or
pfe% aws_qdel --group gid jobid.clpbs-01.nas.nasa.gov
```

Location of Your PBS Output/Error Files

Within a few minutes after your job has completed or been terminated, the PBS output/error files are sent back to your \$PBS_O_WORKDIR (where you submitted the job from) on Pleiades.

AWS Job Accounting

AWS charges for the compute instances (CPU/GPU), filesystems, storage, and network for transferring data out of AWS. NAS charges an overhead cost, which is a percentage of the total AWS charge. The Job Costs entry includes both the AWS charge and the NAS overhead charge.

Example Job Accounting Summary

```
Job Resource Usage Summary for 3552.clpbs-01.nas.nasa.gov
Total Runtime : 00:03:03
Job Stage In Time (free) : 00:00:00
Job Startup Time : 00:01:03
Time Spent In PBS Script : 00:02:00
Job Stage Out Time : 00:00:00
Walltime Requested : 02:00:00
Execution Queue : AWS Cloud
Charged To : cstaff
Job Finished : Wed Jul 3 10:38:09 2019
Instance Types (ondemand): 1 m5.xlarge
EBS Usage : 8577331200 bytes
S3 Usage : 0 bytes
Charged Bandwidth Usage : 0 bytes
NAS overhead charge : 0.000 percent
Job Costs : $0.00981639861027
```

Managing PBS Jobs Launched from an AWS Dynamic Front End

This article provides information on managing your PBS jobs submitted from an <u>AWS dynamic</u> front end.

For additional information, see also, Managing AWS PBS Jobs From a PFE.

Note: The aws_pbs_host, aws_qstat, and aws_qdel scripts described in this article are located under /u/scicon/tools/bin on Pleiades. The instructions below assume that you have included /u/scicon/tools/bin in your \$PATH.

After launching and using SSH to access an AWS dynamic front end, you can manage PBS jobs as follows.

Finding Available Queues

To find available queues and their limits, use the -q or -Q option:

```
aws% qstat -q
or
aws% qstat -Q
```

Among the queues listed in the output, you have direct access only to the *cloud* queue, which routes the job to the execution queue *cloud_exec*. The other queues, such as *frontend* and *s3op*, are used by NAS-controlled scripts (*aws_fe and nas_s3_xxx*) for managing the <u>AWS dynamic front end</u> and <u>data at AWS S3</u> on your behalf.

Submitting Jobs (qsub)

You can submit both interactive and batch jobs to the 'cloud' gueue, using:

```
aws% qsub -I -q cloud -lselect=1...
aws% qsub -q cloud job_script
```

Note: You should be able to tell by the hostname included in the prompt whether you are in the front end (awsfe-XXXXX) or in the interactive PBS session (compute-XXXXX).

Note: The wall-time requested for an interactive PBS session should not be longer than the remaining time of your AWS dynamic front-end session.

Checking Jobs (qstat or aws_qstat)

You can check the job status either by using qstat on your AWS front end or by using aws_qstat on a PFE, as follows:

• On the AWS Front-End

```
aws% qstat -a
aws% qstat -nu your_user_name

• On the PFE

pfe% aws_qstat -a @`aws_pbs_host`
pfe% aws_qstat -a @`aws_pbs_host --group gid`(to check a job for a non-default GID)
pfe% aws_qstat -nu your_user_name@`aws_pbs_host --group gid`
```

Deleting Jobs (qdel or aws qdel)

You can delete a job using qdel on your AWS front end or aws qdel on a PFE.

On the AWS Front-End

```
aws% qdel jobid
• On the PFE

pfe% aws_qdel jobid (note, the jobid here is just the numerical part)
pfe% aws_qdel --group gid jobid (to delete a job for a non-default GID)
pfe% aws_qdel --group gid jobid.your_aws_pbs_server
pfe% aws_qdel --group gid jobid.your_aws_pbs_server.nas.nasa.gov
```

Finding Your PBS Output/Error Files

When a job exits, the PBS output file (which includes job accounting data) and error files are placed in the \$PBS_O_WORKDIR on AWS, they are *not* sent back to Pleiades.

Handling Job Accounting

AWS charges for the compute instances (CPU/GPU), filesystems, storage, and network for transferring data out of AWS. NAS charges an overhead cost, which is a TBD percentage of the total AWS charge. The Job Costs entry includes both the AWS charge and the NAS overhead charge.

Example Job Accounting Summary

```
Job Resource Usage Summary for 3622.your aws pbs server.nas.nasa.gov
   Total Runtime
                       : 00:04:10
   Job Stage In Time (free) : Submitted from AWS, no stage in
   Job Startup Time : 00:02:05
   Time Spent In PBS Script: 00:02:03
   Instance Types (ondemand): 1 m5.2xlarge
                       : 16773959680 bytes
   FBS Usage
   S3 Usage
                        : 0 bytes
   Charged Bandwidth Usage : 0 bytes
   NAS overhead charge : 0.000 percent
                        : $0.0268173415057
   Job Costs
```

Staging Between Pleiades and AWS within PBS Jobs Submitted from a PFE

This article describes how to use **stagein** and **stageout** directives in a PBS job script to copy files between Pleiades and the \$PBS_O_WORKDIR directory in AWS.

When you submit a job from Pleiades, the value of the job's \$PBS_O_WORKDIR variable (the cwd at the time of the qsub operation) is recreated in AWS. If the job uses your persistent /nobackup directory, it will be under that filesystem. Otherwise, the value will be a symbolic link created under the node's root filesystem that points to the primary job-time filesystem. This enables the job to change (cd) to the \$PBS_O_WORKDIR directory.

For jobs submitted from Pleiades, the \$PBS_O_WORKDIR is restricted to one under your /nobackup directory, since you can only submit batch jobs to AWS from a Pleiades /nobackup directory.

```
#CLOUD -stagein_file=path_to_file/file
#CLOUD -stagein_dir=path_to_dir
#CLOUD -stageout_file=path_to_file/file
#CLOUD -stageout_dir=path_to_dir
#CLOUD -stageout_file_delete=path_to_file/file
#CLOUD -stageout_dir_delete=path_to_dir
```

Note: In a PBS script, all PBS directives should be specified before the CLOUD directives.

More details about staging are described below:

Using the stagein Directive

You can **stagein** files or directories under your Pleiades /nobackup directory, but not under your Pleiades /home directory.

All Pleiades files to be used in AWS must be specified in the PBS script. You can give individual files (wildcards included) or individual directories.

TIP: If you have a lot of files to stage in, you can tar up the directory, and just stage in the tar file. This will speed up the process. (You will need to untar the file inside your PBS script.) You can use either an absolute or a relative path. When a relative path is used, it is relative to the \$PBS_O_WORKDIR directory on Pleiades where the qsub command was issued.

The staged-in files and/or directories will have the same directory structure on AWS as they have on Pleiades. In the two examples below, the PBS job is submitted from /nobackup/username/run on Pleiades.

Example 1

The following directive will result in /nobackup/username/run/input/file on Pleiades to be staged into /nobackup/username/run/input/file on AWS, not /nobackup/username/run/file on AWS:

```
#CLOUD -stagein file=input/file
```

Example 2

The following directive will copy /nobackup/username/src/mpi_pi.f from Pleiades to /nobackup/username/src/mpi pi.f on AWS:

```
#CLOUD -stagein file=/nobackup/username/src/mpi pi.f
```

Using the stageout Directive

Only the relative path should be used. In addition, staging out files to Pleiades at a relative path above \$PBS_O_WORKDIR (such as ../src) is not supported. The staged out files and/or directories will have the same directory structure on Pleiades as they have on AWS.

Stageout and Delete

Optionally, you can use the following directives to perform two tasksa stage out, then delete:

```
#CLOUD -stageout_file_delete=output
#CLOUD -stageout_dir_delete=test_dir
```

Order of Operation

- -stagein file and -stagein dir operations occur in the PBS prologue.
- -stageout_file and -stageout_dir operations occur at the end of job, specifically:
 - ◆ For AWS filesystems with a distinct filesystem server, such as a persistent filesystem or a shared-type <u>job-time filesystem</u>, the operations occur on the filesystem server after the job exits.
 - For other types of job-time filesystems, the operations occur in the PBS epilogue.

If you are using other **cLoub** directives, see <u>Order of Operation of Cloud Directives</u>.

Transferring Files Between a Pleiades or AWS Front End and AWS S3 Storage

This article describes how to use the mas_s3_xxx set of commands on a Pleiades front end (PFE) or an <u>AWS dynamic front end</u> to view, transfer, and delete files and directories under your AWS S3 root location (i.e., /).

Similar to the Lou mass storage system at NAS, the AWS S3 system functions as long-term storage. The data stored in your S3 folder is not accessible or visible to any other user. You will not have the required AWS credentials to directly access the S3 storage from either a PFE or an AWS dynamic front end, but you can use the following set of commands to check, transfer or delete files in your S3 folder from a PFE or from an AWS dynamic front end.

On Pleiades, these commands are located in the /u/scicon/tools/bin directory. On an AWS dynamic front end, they are located in the /opt/pbs/bin directory.

Note: To use these commands, you must have write permission on the location where the commands are issued.

- View: nas_s3_ls [--group X] my_folder
- Transfer to S3: nas_s3_put [--group X] [file1 directory1 file2 directory2 ...] s3_folder
- Transfer from S3: nas s3 get [--group X] [file1 folder1 file2 folder2 ...]
- Delete: nas s3 del [--group X] [file1 file2 folder1 folder2 ...]

If you have more than one AWS group, and you want to use a non-default one, add --group X where X is a group ID (GID).

Please note the following:

- A nas_s3_xxx command creates a PBS job to the s3op queue behind the scenes. It may take a few minutes to get a response back after issuing the command. After putting files/directories to S3 with the nas_s3_put command, it may take up to 10 minutes to see them at S3 with the nas s3 ls command.
- Currently, there is a limit of 10 nas_s3_xxx jobs per user. Pending usage loads and network bandwidth, the limit may change in the future.

To learn more and find examples, simply issue any one of these commands without any options on a PFE or an AWS dynamic front end.

Transferring Files Between AWS S3 Storage and Your AWS PBS_O_WORKDIR Directory

Use the **CLOUD** directives described in this article to copy files between your S3 storage on AWS and your \$PBS_O_WORKDIR directory in AWS.

When you submit a job from Pleiades, the value of the job's \$PBS_O_WORKDIR variable (the cwd at the time of the qsub operation) is recreated in AWS. If the job uses your persistent /nobackup directory, it will be under that filesystem. Otherwise, the value will be a symbolic link created under the node's root filesystem that points to the primary job-time filesystem. This enables the job to change (cd) to the \$PBS_O_WORKDIR directory.

Note: In a PBS script, all PBS directives should be specified before the **CLOUD** directives.

Get Files or Directories from S3 to \$PBS_O_WORKDIR

The following **CLOUD** directives allow you to get files or directories from the specified S3 folder to the \$PBS_O_WORKDIR directory in AWS.

• To get your dir1/dir2/file in S3 and place it as PBS 0 WORKDIR/dir1/dir2/file:

```
#CLOUD -get file=dir1/dir2/file
```

• To get your dir1/dir2/file in S3 and place it as PBS_0_WORKDIR/dir2/file:

```
#CLOUD -get file=dir2/file:dir1
```

• To get your dir1/dir2/file in S3 and place it as PBS_0_WORKDIR/file:

```
#CLOUD -get_file=file:dir1/dir2
```

 To get all files from your dir1/dir2 directory in S3 and place them under PBS 0 WORKDIR/dir1/dir2:

```
#CLOUD -get dir=dir1/dir2
```

 To get all files from your dir1/dir2 directory in S3 and place them under PBS_0_WORKDIR/dir2:

```
#CLOUD -get_dir=dir2:dir1
```

• To get all files from your dir1/dir2 directory in S3 and place them under PBS 0 WORKDIR:

```
#CLOUD -get dir=/:dir1/dir2
```

Example 1

The following command line will get the output.dat file under your S3 run01 directory and place it as \$PBS_0_WORKDIR/run01/output.dat:

```
#CLOUD -get_file=run01/output.dat
```

Example 2

The following command line will get all files under your S3 run02/data directory and place them under \$PBS 0 WORKDIR/data:

```
#CLOUD -get dir=data:run02
```

Put Files or Directories to S3

To put files or directories to S3, run the following commands, where src_file or src_dir is relative to \$PBS_0_WORKDIR and optional_dest_dir is relative to your S3 root location.

```
#CLOUD -put_file=src_file:optional_dest_dir
#CLOUD -put dir=src dir:optional dest dir
```

If optional_dest_dir is not specified, #PBS_O_WORKDIR/src_file is copied to your S3 root location, and \$PBS_O_WORKDIR/src_dir/* is copied to the src_dir/* under your S3 root location.

Example 3

To put \$PBS_0_WORKDIR/data/output.dat as run02/output.dat under your S3 root location:

```
#CLOUD -put_file=data/output.dat:run02
```

Example 4

To put \$PBS 0 WORKDIR/data/hdf5/* as run03/hdf5/* under your S3 root location:

```
#CLOUD -put_dir=data/hdf5:run03/hdf5
```

Order of Operation

The -get_xxx operations occur before the execution of the body of the PBS script, while the -put xxx operations occur after the execution of the body of the PBS script.

If you are using other **CLOUD** directives, see <u>Order of Operation of Cloud Directives</u>.

Creating AWS Job-Time Filesystems

A job-time filesystem is created at the beginning of each PBS batch job submitted from either a Pleiades front-end system (PFE) or an AWS dynamic front end. The filesystem is maintained while the job is running. When it is terminated at the end of the job, the data in the filesystem is lost. You are charged for the size provisioned for the lifetime of the job and the uptime of the filesystem server (if needed).

Note: Job-time filesystems are not created for interactive PBS jobs submitted from an <u>AWS</u> dynamic front end.

Adding the CLOUD Directives to Your PBS Script

Use the following directives in your PBS script to create various types of job-time filesystems, and to specify the size and mount point:

```
#CLOUD -volume_type=type
#CLOUD -volume_size=size_in_GB
#CLOUD -volume_mount=/path/to/mount/on
```

Important: The CLOUD directives must be placed after the the PBS directives in a PBS script.

-volume_type

The -volume_type directive must be placed before the â volume_size and â volume_mount directives in the PBS script; before â volume_put and â volume_get, which are described in this article; and before â volume_primary, which is described in this article.

See the next section for a list of options you can specify for the â volume type directive.

-volume size

For -volume_size, a number in gigabytes (G) is expected; any unit you add to it is ignored. For example, each of the following three specifications results in a request for a volume size of 10 G:

```
#CLOUD -volume_size=10
#CLOUD -volume_size=10G
#CLOUD -volume_size=10T
```

-volume mount

For -volume_mount, mounting as /home is not currently allowed.

You can use as many sets of job-time filesystems as you want for each job. However, to reduce complexity for your job, we recommend using a maximum of two.

Types of Job-Time Filesystems

There are several types of job-time filesystems you can configure for your job. Some factors to consider when choosing a type are I/O pattern, size, performance, and cost.

You can specify the following options for the â volume type directive:

• ephemeral

Uses the ephemeral Non-Volatile Memory Express (NVMe)-based Solid State Drive (SSD) space that is local to various computing instance types. This type will ignore the **a** volume size setting because the local space determines the size available.

Not all instance types have a local disk. If the type you specify doesn't have disks available, it ignores the directive.

For best results using NVMe-based SSD, add arch=c5d into the select line in the PBS script, as that is the only instance type currently supported by NAS. Note that c5d comes in six sizes, with 1, 2, 4, 8, 19, and 36 physical cores, and up to 1,800 GB of NVMeâ based SSD.

• local

Each computing instance gets its own unique EBS filesystem. The size of the EBS volume unique to each computing instance is determined by $\hat{\mathbf{a}}$ volume_size=x. The x GB EBS volume accessed by one computing instance cannot be accessed by another computing instance, which has its own x GB of EBS to use.

headnode

Only the head node gets the EBS volumes. The size of the EBS is determined by the **a volume_size**. Other computing instances do not have access to the EBS on the head node.

• node=x

The xth computing instance gets an EBS filesystem. Specifying node=0 has the same result as specifying headnode. The EBS filesystem of this xth instance is not accessible by another instance.

shared

Creates a distinct filesystem server instance that NFS-exports the volumes to all computing instances. None of the computing instances is used as the filesystem server.

To select an instance as a filesystem server, it first looks at the â volume_size request. If there is an instance type that has at least the amount of local spaceâ NVMe SSD or Hard Disk Drive (HDD)â requested, that instance will be selected over other instances with EBS mount storage. Otherwise, a c5.18x instance with added EBS volumes to satisfy the required space will be selected.

In other words, this "shared" filesystem has a few options for instances it will select behind the scenes. For the following requested volume sizes:

- ♦ Under 1.8 TB: a c5d.18x instance with local SSD disks is selected.
- Between 4 TB and 16 TB: an h1.16x instance with local HDD disk is selected.
- For any other size: the normal c5.18x instance with EBS volumes is selected.

headnode

The EBS volumes on the head computing instance are NFS-exported to all other computing instances.

Note: Exporting ephemeral space, if any, on the head computing instance to other computing instances is currently not supported by the NAS cloud developers.

lustre

Creates a distinct filesystem using Amazon FSx for Lustre. The size will be determined by the value of -volume_size. There is an AWS-imposed minimum size of 3,600 GB. This filesystem will be mounted on all compute nodes at the mount point specified by a volume_mount.

Note: Using this filesystem will delay job startup by a few minutes while the filesystem is created.

For examples of how these directives are used, see this article.

Transferring Files Between AWS S3 and Job-Time Filesystems

Use these **CLOUD** directives to copy files between your <u>job-time filesystems</u> on AWS and your S3 storage on AWS.

```
#CLOUD -volume_put=s3_folder_name_to_copy_to
#CLOUD -volume_get=s3_folder_name_to_copy_from
```

Please note the following:

- All **CLOUD** directives should be placed after the PBS directives in a PBS script.
- The -volume_put and -volume_get directives should be placed after the â volume_type directive in a PBS script, and can be placed either before or after the â volume_size and â volume mount directives of the corresponding job-time filesystem.
- No leading slash should be used in the s3_folder_name, as demonstrated in the example in this section.
- The S3 folders are all relative to your S3 root location (i.e., /). Other users, even those in the same group, cannot see your files in S3.
- The -volume_get directives will get everything inside the specified folder. Getting a single file from an S3 folder is not currently supported.

If you give the **-volume_put** directive for a job-time filesystem where multiple nodes have their own space (such as the *ephemeral* or *local* type of filesystem, but not the *shared* type), then files from all of the nodes will be put in the same S3 folder. This results in files with the same name on each node ending up in an undetermined state as to which node's version is stored. You can avoid this by including {node} in the S3 folder name, so the path will have nodeX appended to it when saved on the X node's copy. For example, for a job that asks for three nodes with these directives:

```
#CLOUD -volume_type=local
#CLOUD -volume_put=run12/{node}
#CLOUD -volume mount=/data
```

the following directories in your S3 environment will be created and files in the /data/ directory from each node will be stored in the appropriate one:

```
/run12/node0
/run12/node1
/run12/node2
```

The -volume_get directive works similarly in these situations, but without the need for the {node} text.

For a filesystem type that is unique to each node (for example, ephemeral, local, headnode, or node=X), if the number of nodes used in the 'put' operation is less than the number of nodes used in the 'get' operation, then some nodes may have empty directories from the 'get' operation. However, if the number of nodes used in the 'put' operation is more than those in the 'get' operation, then not all the data from the 'run12' S3 bucket will be brought back.

For more information, see:

- Examples of Job-Time Filesystem Related Directives
- Optional Job-Time Filesystem Related Directives

Order of Operation

- The -volume_get operation happens when the compute instance boots.
- The -volume_put operation for shared filesystems occurs after the job exits, and therefore will not show up in the output of â volume_list (if included in the job script). You can use the nas s3 ls command (described in this article) to see them in S3 afterwards.
- The -volume_put operation for non-shared filesystems occurs after the PBS script but before the â volume_list operation.

If you are using other **CLOUD** directives, see <u>Order of Operation of Cloud Directives</u>.

Optional Job-Time Filesystem Related Directives

This article describes optional AWS Cloud directives to use in addition to those for creating a <u>job-time filesystem</u> and those used for <u>transferring files between S3 and a job-time filesystem</u>.

• -volume include

By default, jobs will not have persistent, shared /home and /nobackup filesystems mounted if there are any â volume_type directives given. Without a persistent /home filesystem mounted, you will get an empty /u/username directory as part of the root filesystem on the node.

The -volume_include option can be used to indicate that you want to have the persistent /home and/or /nobackup mounted as normal.

```
#CLOUD -volume_include=home
#CLOUD -volume_include=nobackup
```

Important: If the persistent /home or /nobackup filesystems are mounted, those two paths are not available as a mount destination for job-time filesystems.

The -volume_include directive, together with a stagein_file/dir and a stageout_file/dir used to stage in/out files between Pleiades and AWS can be placed above the first a volume type directive.

• -volume_home_{bashrc,profile,login,cshrc}

```
#CLOUD -volume_home_bashrc=local_file
#CLOUD -volume_home_cshrc=local_file
#CLOUD -volume_home_profile=local_file
#CLOUD -volume_home_login=local_file
```

These directives will take the given file in the current directory (i.e., \$PBS_O_WORKDIR) and make it the ~/.bashrc (or .cshrc, .profile, .login, depending on which specific directive is used) to be automatically sourced under \$HOME at job startup for all instances. In the event there isn't an existing persistent shared /home used, the .bashrc will be placed under each instance's empty /home under the root filesystem. This will allow some control over the environment for things that can't be set in the PBS script (i.e., variables on the nonâ headnode).

These directives can be placed above the first â volume_type directive.

Note: The default shell is bash unless you have requested changing it. If you want to use csh and have the .cshrc sourced in a PBS job, add the following to the beginning of your PBS script:

```
#PBS -S /bin/csh
• -volume_primary
```

In the event that there are multiple filesystems mounted in a job, you can use this directive to toggle a filesystem on as the source and destination for â get_file, â put_file, â stagein_file/dir, and â stageout_file/dir, and also to create a softlink for \$PBS O WORKDIR to the following primary filesystem:

```
#CLOUD -volume primary
```

This directive should be placed anywhere before the specification of the next filesystem block that starts with â volume_type.

However, if a persistent /nobackup filesystem is mounted, it is set as the primary regardless of whether any job-time filesystem has -volume_primary set. Conversely, a persistent /home filesystem cannot be set as primary.

If more than one job-time filesystem is specified as the primary, the first one specified with â volume_primary is chosen.

If there is no user-indicated primary, the system picks the first one that exists in this order:

```
shared
lustre
headnode_shared
headnode
node=X
local
ephemeral
```

For example, the following specification will result in /shared 1 as the chosen primary.

```
#CLOUD -volume_type=headnode
#CLOUD -volume_mount=/data
..
#CLOUD -volume_type=shared
#CLOUD -volume_mount=/shared_1
..
#CLOUD -volume_type=shared
#CLOUD -volume_mount=/shared_2
•-volume list and -volume delete
```

These two options can be used to see the contents and to remove, if desired, any previously 'put' filesystems. They can be placed anywhere after the #PBS directives.

```
#CLOUD -volume_list=s3_folder_to_list
#CLOUD -volume delete=s3 folder to remove
```

The -volume_list and -volume_delete operations occur after the execution of the PBS script. Read this article for more information.

Examples of Job-Time Filesystem Related Directives

This article provides a few examples of how the job-time related CLOUD directives are used.

Please review the following articles before you begin using the examples shown below:

- Creating a job-time filesystem
- Transferring files between S3 and a job-time filesystem
- Optional job-time filesystem related directives

Using Local Job-Time Filesystems

Data written to a local disk of a node are not accessible to processes running on other nodes. One scenario where the usage of such local disks is appropriate: running a CFD application where its MPI processes write out one file per rank or per node and the file is not needed by other ranks or nodes. The following examples walk you through this scenario.

Examples 1 and 2 show how to utilize the job-time local disks (/data, shown in the examples) for staging in the executable file (a.out) and input file (input.dat) from the Pleiades /nobackup system; and how to store rank-identified restart files generated by individual ranks in separate node-identified sub-folders of AWS S3 at the end of a job.

In Example 1, the ephemeral volume type is used when the local space needed for the restart file is less than 1.8 TB. In Example 2, the local volume type is used when the space needed is more than 1.8 TB.

In Example 3 (after you have followed the steps in Example 1 or Example 2), the restart files are loaded back from the S3 sub-folders to the local disk to resume simulation.

Note: If you do not store the restart files into sub-folders according to node numbers, when it is time to load the files back for the next job, each node will get all the restart files instead of just the ones needed for the ranks on the node.

Example 1

Specifying arch=c5d allows c5d.18x instances with 1.8 TB of NVMe SSD to be used as local disks.

```
#PBS -l select=10:mpiprocs=36:arch=c5d
...
#CLOUD -volume_type=ephemeral
#CLOUD -volume_put=outputfolder/{node}
#CLOUD -volume_mount=/data
...
#CLOUD -stagein_file=a.out
#CLOUD -stagein_file=input.dat
...
cd /data/
mpiexec -np 360 ./a.out < input.dat</pre>
```

Example 2

If you space needs more than 1.8 TB of space for the restart files, then specify the local volume

type and a large volume size (for example, 2,048 GB).

```
#PBS -l select=10:mpiprocs=36:arch=c5d
...
#CLOUD -volume_type=local
#CLOUD -volume_put=outputfolder/{node}
#CLOUD -volume_mount=/data
#CLOUD -volume_size=2048
..
#CLOUD -stagein_file=a.out
#CLOUD -stagein_file=input.dat
..
cd /data/
mpiexec -np 360 ./a.out < input.dat</pre>
```

Example 3

Since the **-volume_put** directive was included when the previous job was done (as shown in examples 1 and 2), the files got saved off for this follow-on job to start from.

The -volume_get directive will bring back the files into the corresponding node in this new job. You do not need to include {node} in the get directive.

```
#PBS -l select=10:mpiprocs=36:arch=c5d
...
#CLOUD -volume_type=ephemeral
#CLOUD -volume_get=outputfolder
#CLOUD -volume_put=outputfolder
#CLOUD -volume_mount=/data
...
#CLOUD -stagein_file=a.out
#CLOUD -stagein_file=input.dat
...
cd /data/
mpiexec -np 360 ./a.out < input.dat</pre>
```

Using Shared Job-Time Filesystems

Example 4 shows how to create a filesystem (/nobackup, in this example) that only exists for the duration of the job and is shared by all nodes.

Example 4

```
#PBS -l select=10:mpiprocs=36
...
#CLOUD -volume_type=shared
#CLOUD -volume_size=2048
#CLOUD -volume_mount=/nobackup
...
cd /nobackup
mpiexec -np 360 ./a.out < input.dat</pre>
```

The directives -volume_put and -volume_get can be used if you want to save files in S3 between runs.

Example 5

If your job is such that the head node/rank does most of the writing, but there are some files that all ranks need to see, the headnode_shared volume type is useful.

```
#PBS -l select=10:mpiprocs=36
..
#CLOUD -volume_type=headnode_shared
#CLOUD -volume_size=2048
#CLOUD -volume_mount=/nobackup
...
```

Using Both Shared and Local Job-Time Filesystems

Example 6

Certain jobs may have some ranks that perform CFD computations and some that handle I/O or mesh regridding and need local disk space. You can use a shared filesystem for the computation and the node=X volume for those ranks that need local disk space. For example, if rank 10 and rank 50 need space but not the others, you can use:

```
#PBS -l select=10:mpiprocs=10
...
#CLOUD -volume_type=shared
#CLOUD -volume_size=100
#CLOUD -volume_mount=/nobackup
...
#CLOUD -volume_type=node=1
#CLOUD -volume_size=512
#CLOUD -volume_mount=/data
...
#CLOUD -volume_type=node=5
#CLOUD -volume_size=512
#CLOUD -volume_mount=/data
```

In this case, only node 1 and node 5 will have extra space in /data. The other nodes will use the shared filesystem, /nobackup.

Using a Non-Default Startup Script

Example 7

A job startup script under \$HOME is useful to provide a customized environment for a login session or for different nodes in a PBS job. The customized environment may include the module load commands or set certain environment variables.

If the job does not use the persistent /home shared filesystem, where a startup script may be available, you can provide one that is accessible from the job's \$PBS_O_WORKDIR, to be used in the place of the \$HOME startup script. You can tell PBS to use that file instead of the system default ~/.bashrc file created on each compute node at boot time, as follows:

```
...
#CLOUD -volume_home_bashrc=my_bashrc_file
```

Order of Operation of Cloud Directives

In situations where you have files with the same filename but with different contents in different places--such as on Pleiades, various folders of AWS S3, and various job-time filesystems--pay attention to the executation order shown below to avoid unintentionally getting or putting, or using or deleting the wrong copy.

Please review the following articles to understand the overall operation of the HECC cloud environment:

- Staging between Pleiades and AWS within PBS
- Transferring files between AWS S3 and \$PBS O WORKDIR
- Creating a job-time filesystem
- Transferring files between AWS S3 and job-time filesystems
- Optional job-time filesystem related directives

Order of Execution

- Persistent filesystems:
 - 1. -stagein file/ dir
 - 2. -get_file
 - 3. -volume home {bashrc,profile,login,cshrc}
 - 4. pbs script
 - 5. (-put_file/-stageout_file/_dir)
 - 6. -volume list
 - 7. -volume delete
- "Shared" type job-time filesystems:
 - 1. -volume get
 - 2. -stagein file/ dir
 - 3. -get file
 - 4. -volume home {bashrc,profile,login,cshrc}
 - 5. if primary then -stagein file/ dir and -get file
 - 6. pbs script
 - 7. -volume list
 - 8. -volume delete
 - 9. -put file
 - 10. -stageout file/ dir
 - 11. -volume put
- Non-"shared" type job-time filesystems (node, local, ephemeral, master_shared):
 - 1. -volume_get
 - 2. -volume_home_{bashrc,profile,login,cshrc}
 - 3. if primary then -stagein_file/_dir and -get_file
 - 4. pbs script
 - 5. -volume put
 - 6. (-put file/-stageout file/ dir)
 - 7. -volume list
 - 8. -volume delete

The (-put_file/-stageout_file/_dir) is in the order that the directives exist in the PBS script.

The -volume_get operation happens when the compute instance boots up. For the -volume_put operation, it depends on the filesystem used:

• "Shared" filesystems: Done on the filesystem server after the job exits.

• All other filesystems: Done on the filesystem after the PBS script and before the -volume_list operation.

WARNING: It is recommended not to delete a folder in which you intend to 'put' files within the same PBS job.

Cloud Billing Units and Accounting

Usage on the HECC AWS Cloud is charged in Cloud Billing Unit (CBU) where 1 CBU = 1 US dollar. A project is given an allocation of N CBUs when the principal investigator (PI) provides his/her NASA Work Breakdown Structure (WBS) number with N US dollars.

Charges include the following categories:

AWS Dynamic Front End Usage

A charge to the user for using the AWS dynamic front end is recorded on a per-front-end-request basis. After the front end session is terminated, an email with the charging record is sent to the user (see <u>AWS dynamic front end</u> for an example email). This charge is reflected in the <u>acct query output</u> under the frontend queue.

PBS Jobs Usage

A charge to the user for running a PBS job is recorded on a per-job basis. After the job is terminated, the charging record is included in the PBS output file, which is sent to the \$PBS_O_WORKDIR. For jobs submitted from a PFE, the \$PBS_O_WORKDIR is under the user's Pleiades /nobackup directory. For jobs submitted from an AWS dynamic front end, the \$PBS_O_WORKDIR is a directory on an AWS filesystem (a sample output can be found at the end of this article). This charge is reflected in the acct_query output under the cloud exec queue.

nas_s3_{get,ls} and Per-User S3 Long Term Storage Usage

Charges associated with per-user and/or per-job S3 usage such as running the nas_s3_{get,ls} commands from NAS (which incur both file-transfer-out of AWS and network costs) and storing data in S3 are recorded daily with no individual notification in the form of an email or per-job output. They are reflected in the acct_query output under the daily resource charge (drc) queue.

PBS Server at AWS, Job-Time Filesystem of -volume_type=shared, Persistent Filesystems, and Project-Level S3 Storage Usage

A charge to the PI for using resources that cannot be accounted for on a per-job and/or per-user basis is recorded on a per-day basis. The record of these charges is only available through <u>acct query</u> under the drc queue for the PI.

AWS Project Account Charge

In order to comply with NASA rules and regulations for working in the cloud, there are a number of underlying resources active in the project's AWS account. These cannot easily be included on a per-PBS-job or per-day basis, so they are added at the end of the month when the final AWS bill arrives. The charge normally amounts to ~\$100/month and it is not reflected in the acct_query output.

NAS Overhead

In addition to the hardware and network resources, there is support infrastructure by AWS and HECC to be maintained. An overhead cost for this infrastructure is added to the charges for the above items.

Allocation Thresholds

Allocations are checked once a day at 12:05 a.m. (Pacific Time). When a project's allocation goes below a certain threshold, the GID and its users are disabled in the PBS Access Control List (ACL). Re-enabling happens automatically at 12:05 a.m. if the allocation goes above the threshold after the PI sends in additional funding. In the event the PI wants his/her account to be reactivated immediately, NAS staff with root privilege can also run a script at anytime to update the ACL.

Use the acct_ytd and acct_query tools on a PFE to check your allocation usage on AWS (-caws) or all supported HECC Cloud providers (-ccloud-all). For example,

```
pfe% acct_ytd -caws
pfe% acct_ytd -ccloud-all
pfe% acct_query -caws -u username -p your_gid -b 07/01/19
pfe% acct query -ccloud-all -u all -p all -b 07/01/19
```

A sample output of the last command is shown here:

```
Printing information for all the users supplied. REPORT FROM 07/01/19 TO 07/19/19
```

ACCT QUERY: Generating data ...

GRAND TOTAL FOR G	7/01/19 TO (PROJECT	07/19/19 QUEUE	SBU Hrs/Cloud BU
aws staff1 aws staff1 aws staff1 aws staff2 aws staff2 aws staff2 TOTAL FOR aws.	cstaff cstaff cstaff	cloud_exec drc frontend cloud_exec drc frontend	2.207 6.000 73.781 2.337 0.000 5.821 90.146
TOTAL FOR ALL PROJECTS FOR CLIENT: aws TOTAL FOR PROJECT ON ALL CLOUD: cstaff			90.146 90.146

Note: All numbers shown in the output of acct_ytd and acct_query for HECC AWS Cloud usage are in CBUs.

AWS PBS Resources and Examples

This article lists the qsub command options that are specific to the HECC AWS Cloud, and provides examples showing how to use them.

Accepted Resource Attributes

You can use these attributes for the -1 select option:

```
: minimum n cores per node
mpiprocs=n: n MPI processes per node
         : minimum n GB of RAM per node; can be simply nG, ng, or nM, nm.
arch=xx
        : specifies an architecture type
             If not specified, the cheapest instance type
             that satisfies the user's request will be
             chosen automatically.
             most common ones are: c4/c5/m4/m5
             c4 allows for up to 18 cores and 60G per node
             c5 allows for up to 48 cores and 192G per node
             m4 allows for up to 32 cores and 256G per node
             m5 allows for up to 48 cores and 384G per node
        : To specify the GPU node type.
qpu=xxx
             xxx should be either k80 or v100.
             The K80 nodes have either 1, 8, or 16 GPUs per node
            The V100 nodes have either 1, 4 or 8 GPUs per node
napus=n
         : minimum n gpus per node
net=x
         : Target network bandwidth in/out of node.
             Options supported are 1, 10, 25.
             Not specified will allocate a node type based
             on other specified resource requests only.
             If specified will allocate (if possible)
             a node type that satisfies other requests and:
             net=1 -> can sustain around 1+ Gbps.
             net=10 -> can sustain 10 Gbps
             net=25 -> can sustain 25 Gbps
```

The following PDFs list the CPU and GPU node types that are supported in AWS:

- CPU node types (PDF)
- GPU node types (PDF)

In all regions of AWS, on-demand nodes are used by default. Spot nodes are generally significantly less expensive then on-demand nodes. The drawback is that spot nodes are subject to being taken away based on AWS load and are not always available.

To request spot nodes for your cloud job, use the cloud_model directive in your PBS script:

```
#CLOUD -cloud_model=[spot, onlyspot]:block
```

- Specifying the type "spot" will indicate that the job should start using spot instances; if there are not enough spot resources for the job, it will transfer over to an on-demand job type.
- Specifying the type "onlyspot" will indicate that the job should start using spot instances; if there are not enough spot resources, the job will fail.
- The optional value ":block" indicates you want all instances to fail if any single instance is taken away.

For example, the following line will try to start the job on spot instances; if that isn't possible, it will try to start them as on-demand instances. If any of the spot instances is taken away by AWS, the entire job will be terminated:

```
#CLOUD -cloud model=spot:block
```

On-demand jobs can also fail if resources are not available in AWS. Jobs are automatically retried 10 times before failing due to insufficient resources.

Note: In the PBS script, a **CLOUD** directive should be placed after all PBS directives have been specified.

Job Dependencies

We do not recommend submitting a job (Job B) that depends on another job (Job A), such as -W depend=afterany:job_id.server_name.nas.nasa.gov, because resources for Job B may be grantedâ and charging for Job B may beginâ before Job A terminates or completes, and before Job B actually executes.

Rerunning Jobs

Jobs submitted to run on the AWS cloud cannot be rerun by PBS, no matter what causes the job to fail. Specifying #PBS -r has no effect.

Resource Request Examples

• To request 2 nodes with a minimum of 2 cores and 16g of memory:

```
#PBS -l select=2:mpiprocs=2:ncpus=2:mem=16g
```

To reguest 3 c4 nodes each with a minimum of 18 cores and 48g of memory:

```
#PBS -l select=3:ncpus=18:mem=48G:arch=c4
```

• To request 2 nodes with at least 1 K80 cards per node:

```
#PBS -l select=2:mpiprocs=2:ncpus=2:mem=16g:gpu=k80:ngpus=1
```

• To request 3 nodes each with a minimum of 14 cores and 4g of memory, plus 2 nodes each with a minimum of 13 cores and 0.5G of memory, and 1 node with at least 3 K80 cards:

```
#PBS -l select=3:mem=4g:ncpus=14+2:mpiprocs=13:mem=512M+1:gpu=k80:mem=16G:ngpus=3
```

• To request 8 nodes, each with 8 V100 GPUs:

```
#PBS -l select=8:mpiprocs=2:ncpus=2:mem=16g:gpu=v100:ngpus=8
```

Using Jupyter Notebook or JupyterLab in the AWS Cloud

You can run a Jupyter notebook in an AWS front-end instance or in a PBS batch job, with either GPU or non-GPU instances.

Before You Begin: To use this capability, you must set up SSH passthrough and SSH port forwarding from your local system to a Pleiades front-end system (PFE) and then to an AWS node. If you need help to set these up, send an email with your contact information to support@nas.nasa.gov.

Running a Jupyter Notebook or JupyterLab in an AWS Front-End Instance

When you start an AWS front-end instance, add either the --jupyter or the --jupyterlab argument to the aws_fe command. For example, to start a Jupyter notebook or JupyterLab on an instance with a single NVIDIA Tesla V100 GPU card, run:

```
pfe: module load scicon/aws_cli_tools
pfe: aws_fe --group cloud_gid --hour 5 --gpu=v100 --jupyterlab
or
pfe: aws fe --group cloud gid --hour 5 --gpu=v100 --jupyterlab
```

When the instance starts, you will be sent an email with instructions describing how to connect and point your local browser to the Jupyter login page.

By default, a token is used for authentication when connecting to the Jupyter web interface. You can obtain this token by running the following command on the AWS front-end instance:

For Jupyter Notebooks:

```
aws: jupyter notebook list
```

For JupyterLab:

```
aws: jupyter server list
```

If you prefer to set up a password instead, you can create one while logged into any AWS instance by running the following command:

```
aws: jupyter notebook password
```

You will be prompted for a password, and the file <code>jupyter_notebook_config.json</code> will be created in the <code>/u/username/.jupyter</code> directory. (If this file already exists, an entry will be added to it.)

The most commonly used packages are already installed in the version of Python that Jupyter uses by default. If you want to use different packages, you can set up your own virtual environment for a kernel. For example, because GPU-capable versions of the Python packages are not installed in the default environment, you might want to create your own.

Creating Your Own Virtual Environment

The example below shows how to create a virtual environment to install GPU-capable versions of the Python packages.

TIP: To see a list of Python packages you might want to install, run the module help cuda/10.0 command.

To create your own virtual environment, run:

```
aws: module purge ; module load python/Python3.6
aws: python3 -m venv /u/username/.venv/gpu
aws: module purge
aws: module load cuda/10.0
aws: source /u/username/.venv/gpu/bin/activate
aws(gpu): pip install .. whatever packages you need...
aws(gpu): pip install ipykernel
```

Then, enable Jupyter to see this virtual environment as an option for its kernel by creating this file:

/u/username/.local/share/jupyter/kernels/name/kernel.json

where *name* can be anything, such as the name of your environment. The file should contain the following contents:

Notes:

- The "env" line in the .json file is shown on two lines due to a KB formatting issue. It should be on one line.
- You must load the python3.6 module because the default Python version (v3.7) has issues with the TensorRT packages required for tensorflow-gpu on the system.
- The first item in the argv list is the full path to Python in your virtual environment (venv). Be sure to use /u/username/ instead of '~/'.
- Set the value for display name to anything you like.
- Set the LD_LIBRARY_PATH variable to point to the CUDA libraries if you installed tensorflow-gpu, which needs these libraries. CUDA v10 is the only version that works with the current version of tensorflow-gpu (as of April 2020).

When Jupyter is started, the Python virtual environment (venv) will be available as a kernel option under the **New** dropdown menu.

Running a Jupyter Notebook in a PBS Batch Job

You can start an instance with Jupyter running in a PBS batch job, either from a PFE or an AWS front end. Jupyter running in a batch job will have access to any Python virtual environments and password settings you've added.

In your qsub command line, add the PBS select option service=jupyter to the first node.

For example, from a PFE:

```
pfe: qsub -q cloud@clpbs-01 -l
```

Note: The qsub command line is shown on two lines due to a KB formatting issue. It should be on one line.

From an AWS front end:

```
aws: qsub -l select=1:mpiprocs=14:mem=24:service=jupyter+2:mpiprocs=14:mem=24 script.pbs
```

Note: Jupyter is only started on the head node, even in the following two submission examples:

```
    qsub -l select=3:mpiprocs=14:mem=24:service=jupyter
    qsub -l select=1:mpiprocs=14:mem=24:service=jupyter+2:mpiprocs=14:mem=24:service=jupyter
```

For the following use cases, Jupyter will look at PBS NODEFILE and spawn onto the other nodes:

- If you are using the built-in Dask as the parallel processing tool.
- If you are using any Python packages or tools that understand the Slurm or PBS environments.

To get access to the Jupyter notebook running inside the batch job, be aware that batch job instances are not accessible from outside AWS, but they are accessible from a front end running in AWS. From an AWS front end, there are two possible ways to obtain the URL needed to access Jupyter running on the head node of your batch job.

- If one of the following two files is successfully deposited by the Jupyter server to your \$HOME on AWS, look for the URL embedded in that file:
 - ♦ ~/jupyter output \${PBS JOBID}
 - ♦ ~/jupyter lab output \${PBS JOBID}

Note that this method works only if the compute nodes of your batch job sees your AWS \$HOME as a default shared filesystem.

- Obtain the URL by running the jupyter notebook list command on the head node of your batch job by following these steps:
- 1. On an AWS front end, use the qstat command as shown below to list the PBS jobs running and the head node associated with the job:

```
aws: qstat -W o=+Rank0
```

- 2. Use SSH to connect to the head node in order to access the Jupyter notebook running inside the batch job.
- 3. To get the URL needed to access Jupyter, run the following command on the batch node:

```
aws: jupyter notebook list
```

Running a Singularity Container Image in AWS

In our Amazon Web Services (AWS) environment, Singularity is built into the base compute image (operating system), so you do not need to load a module in order to run a Singularity container in AWS. Normal operation is nearly identical to the Pleiades environment described in Running a Singularity Container Image on Pleiades, with one main difference described below.

Building/Converting SIF Files in AWS

If you want to build your own SIF files, or convert an SIF file into a sandbox image in the AWS environment, you must add the **container=singularity** option to the typical PBS â l select command line. as follows:

#PBS â l select=2:mpiprocs=16:container=singularity:mem=64

This option increases the size of the /tmp filesystem and points the Singularity cache and TMPDIR environment variables to this filesystem. This is helpful both when you build SIF images and when you run them.

Note: When you start a front end in AWS using the aws_fe command, the â â container singularity command line argument provides the same functionality as the container=singularity does in the â l select line.

For more information, see AWS Dynamic Front End.

AWS Cloud FAQs

Can I get more information about your AWS Public Cloud offering?

To learn more about our AWS Public Cloud offering, please watch the 50-minute webinar recording "Overview of HECC Pay-for-Use AWS Cloud," which you can find on the <u>HECC Webinars page</u>.

Also, see our many Knowledge Base articles in the AWS Cloud section.

On a high level, what kinds of work are supported?

The work must be an HPC science or engineering project, whose workflow can be modified to run via a qsub command (in order to submit a batch or interactive job from a NAS front-end system).

Note: A batch job running on the AWS compute instances will have no access to/from NAS or to/from the internet. If your workflow requires the AWS instance be able to access the internet (but not be accessible from the internet), an AWS front-end instance can be launched. Access from NAS to this instance is allowed.

On a high level, what kinds of work are not supported?

We are not currently able to support the following scenarios:

- Enterprise applications that are not HPC-related (for example, Tecplot, MATLAB, and ANSYS are supported while web or eCommerce apps are not).
- Enterprise-level data storage (for example, offsite backups of data via appliances, unless it's a NAS-owned appliance).
- AWS services that don't yet have FedRamp certificationsâ and the demand for a given service is not large enough to justify a request to the NAS security group to allow it.
- User access to the AWS console or command-line interface. (Only certain NAS staff with special privileges can access these.)
- AWS native container technologies.
- Access to resources and/or job submissions from the internet at this time.
- Publicly accessible web pages/S3 storage. This may be allowed in the future.
- Direct access to resources from outside of NAS. This restriction may be removed in the future.

Please check back, as some of these scenarios may be supported in the future.

What CPU and GPU node types are supported in AWS?

The following PDF lists show the CPU and GPU node types that are supported in AWS:

- CPU node types (PDF)
- GPU node types (PDF)

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Is there a way to apply for free access?

We offer a pay-for-use service only. Currently, we do not provide free access. However, the policy may change in the future. Please check back with us from time to time.

We are looking for a cloud environment with software installed. Do you provide Software as a Service (SaaS)?

We currently provide a Platform as a Service (PaaS) cloud environment with a few basic HPC software packages installed (Intel compiler, PGI compiler, Intel MPI, OpenMPI, CUDA, and Python). If you need other software packages, you must install them yourself.

What operating system is used in your cloud?

The default operating system is a basic Linux AWS Machine Image (AMI). Others, such as Red Hat Enterprise Linux (RHEL) or or SUSE Linux Enterprise Server (SLES), can be used upon request. However, the non-default operating system will cost more.

How much does it cost?

The cost will be the same as what you get directly from AWS, plus an overhead cost from NASA Enterprise Managed Cloud Computing (EMCC), where we get our cloud resources. There may also be additional overhead from HECC; this is yet to be determined.

Who do I send my NASA Work Breakdown Structure (WBS) funding?

Please send an email to support@nas.nasa.gov. Our User Services manager will contact you to help you transfer the funding to us.

I do not currently have a NAS account. I can bring funding. How do I start?

After HECC receives your NASA Work Breakdown Structure (WBS) funding, we will guide you in obtaining a NAS account. We will then set up your cloud account.

After my cloud environment is created, how do I log in?

Currently, you will use your NAS account to log into a NAS front end with two-factor authentication. From the NAS front end, you will be able to log into your cloud environment.

Do you allow non-NASA projects to use your cloud offering?

We plan to support collaborative work between NASA and non-NASA scientists. However, this effort is still in a planning stage and will not be in production in 2019. Please do share your

requirements with us so we can better plan to support them.

How do you plan to allow non-NAS users to login to your cloud?

Currently, the HECC cloud can only be accessed from a NAS front-end system. Non-NAS users will be given NAS accounts (without actual HECC allocations) in order to access a NAS front end. This arrangement may change in the future.

Will I be charged if the cloud resources have problems or do not perform as I expected?

Yes. AWS still charges for usage even if your job fails.

Who do I contact if I need help with issues or job failures on AWS?

NAS staff may be able to help you diagnose some issues, but not all. NASA Enterprise Managed Cloud Computing (EMCC) has a support contract with AWS, and therefore some issues can be examined by AWS engineers. However, it is likely some issues won't be resolved easily or quickly.